

Message

From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 8/8/2017 7:10:04 PM
To: Crofton, Kevin [Crofton.Kevin@epa.gov]; Buckley, Timothy [Buckley.Timothy@epa.gov]
CC: Medina-Vera, Myriam [Medina-Vera.Myriam@epa.gov]
Subject: RE: Toxicity?
Attachments: Strynar Nafion like analyte slides 8-7-17.pptx

Here is what we believe the structures to be. See slides 3-end.

Mark

From: Crofton, Kevin
Sent: Tuesday, August 08, 2017 1:03 PM
To: Buckley, Timothy <Buckley.Timothy@epa.gov>
Cc: Strynar, Mark <Strynar.Mark@epa.gov>; Medina-Vera, Myriam <Medina-Vera.Myriam@epa.gov>
Subject: RE: Toxicity?

Tim – I passed this on to Grace. The timeline is rather tight – I will let you know what she says.

Mark – Grace will likely contact you to get a bit more structural information

Kevin

From: Buckley, Timothy
Sent: Tuesday, August 08, 2017 11:14 AM
To: Crofton, Kevin <Crofton.Kevin@epa.gov>
Cc: Strynar, Mark <Strynar.Mark@epa.gov>; Medina-Vera, Myriam <Medina-Vera.Myriam@epa.gov>
Subject: Toxicity?

Kevin,

The two PFCs that appear not to be decreasing in Chemours outfall and downstream source and drinking water (as the case for GenX) are 11 and 12 in the table below. Mark may have additional information to further specify chemical structure. We are planning to provide NC DEQ with these results in the next week or so. In our meeting last week, you indicated that you might be able to say something about toxicity based on read across information. Can you let me know if you might have some assessment of toxicity that you would be willing to share with NC DEQ?

Thanks.

Tim

Table 1. Accurate Mass of Polyfluorinated Compounds and In-Source Artifacts Found in Extracted Water Samples

number	formula	CAS no.	name	[M] ^a	[M - H] ⁻ m/z	[2M - 2H + Na] ⁻ m/z	[2M - H] ⁻ m/z
Monoether PFECAs							
1	C ₃ HF ₅ O ₃			179.9846	178.9773	380.9438	358.9619
2	C ₆ HF ₉ O ₃			229.9813	228.9740	480.9372	458.9553
3	C ₈ HF ₁₁ O ₃	863090-89-5		279.9782	278.9709	580.9310	558.9491
4	C ₈ HF ₁₁ O ₃	13252-13-6	undecafluoro-2-methyl-3-oxahexanoic acid	329.9750	328.9677	680.9247	658.9427
5	C ₇ HF ₁₃ O ₃			379.9718	378.9645	780.9182	758.9363
6	C ₈ HF ₁₅ O ₃			429.9686	428.9613	880.9118	858.9299
Polyether PFECAs							
7	C ₇ HF ₁₃ O ₇	39492-91-6	perfluoro-3,5,7,9,11-pentaoxadodecanoic acid	443.9515	442.9442	908.8776	886.8957
8	C ₆ HF ₁₁ O ₆	39492-90-5	perfluoro-3,5,7,9-butaosadecanoic acid	377.9598	376.9525	776.8942	754.9123
9	C ₅ HF ₉ O ₅	39492-89-2	perfluoro-3,5,7-propaooxooctanoic acid	311.9681	310.9608	644.9108	622.9289
10	C ₄ HF ₇ O ₄	39492-88-1	perfluoro-3,5-dioxahexanoic acid	245.9764	244.9691	512.9274	490.9455
PFESAs							
11	C ₇ HF ₁₃ O ₅ S	66796-30-3 ^b		443.9337	442.9264		
12	C ₇ H ₂ F ₁₄ O ₅ S			463.9399	462.9326		
Other							
	Na ⁺			22.9892			
	H ⁺			1.0073			
	CF ₃ O			65.9917			
	CF ₃			49.9968			

^aIndicates the monoisotopic mass of the neutral species. ^bCAS number for Nafion copolymer.

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Ex. 6 Personal Privacy (PP)